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A Graphical-User-Interface application for multifractal analysis of soil and plant structures

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## ABSTRACT

Multifractal systems are common in nature, and fractal theory has been applied to a large number of patterns for curves, surfaces and volumes in a variety of research domains. For instance, researchers in soil science recently applied multifractal analysis (MFA) to study porosity, which is linked to soil gas diffusion, water content and therefore, nutrient transportation for plants. The calculation of multifractal spectra (singularity, Rényi) is complex and the data can be ‘big’ and of various forms (graphical or numerical), yet the results are highly informative. An easy-to-use GUI-based (GUI: Graphical User Interface) application would allow researchers to concentrate on the results instead of having to deal with the technical aspects. This note fills the gap with the MFA application program, originally written in MATLAB and provided with a user’s guide. Datasets on soil and plant structures (soil porosity, tree branching, biochar structure) are used in three examples, which help illustrate the variety of inputs with our MFA application, demonstrate its generality in performing the MFA method, and interpret the program outputs.

### ***Keywords:***

Soil and plant structures

Multifractal analysis

Singularity spectrum

Rényi spectrum

Graphical-User-Interface application

## 1. Introduction

“Fractals are infinitely complex patterns that are self-similar across different scales. They are created by repeating a simple process over and over in an ongoing feedback loop. Geometrically, they exist in between our familiar dimensions.” (The Fractal Foundation, <https://fractalfoundation.org/resources/what-are-fractals/>)

A plethora of fractal objects and structures exist in the real world. Three examples are considered in this note, all three arising in the 3D space. They are: tree branching (i.e., the very first example listed on the Fractal Foundation website), the porosity of an agricultural soil, and the structure of biochar produced by pyrolysis of wood pellets. Despite some discrepancy between real fractal objects and mathematical ones such as the Mandelbrot Set (Mandelbrot, 1983), fractal analysis has been proven to be very appropriate to quantify the complexity of shapes and patterns from 2D or 3D images (e.g., Burrough, 1981; Foroutan-pour et al., 2001; Dutilleul et al., 2015), including a model goodness-of-fit based on the coefficient of determination in log-log plots of the box- and cube-counting procedures for fractal dimension estimation. Actually, natural structures can be classified as non-fractal and fractal, and subdivided into monofractal and multifractal in the latter class. Multifractal models provide more information about the distribution of a physical system than monofractal models (Voss, 1988), as multifractals allow, through functions called “spectra”, a distribution of the “mass” of interest (pores, branches) over multiple scales and a generalization of dimensions. Two commonly used multifractal spectra are: the singularity spectrum, with parameters  $\alpha(q), f(\alpha(q))$  [rewritten  $f(\alpha_q)$  hereafter] and  $q$  (Chhabra and Jensen, 1989; Evertsz and Mandelbrot, 1992), and the generalized-dimensional spectrum or Rényi spectrum, with parameters  $D_q$  and  $q$  (Grassberger, 1983; Caniego et al., 2003), where  $q$  denotes some moment order in the

equations, or scale. The equations to calculate multifractal mass parameters  $\alpha(q)$ ,  $f(\alpha_q)$  and generalized dimensions  $D_q$  are presented in San José Martínez et al. (2010); see also Lafond et al. (2012) and the Appendix here. A singularity spectrum is a plot of  $f(\alpha_q)$  against  $\alpha(q)$ , and a Rényi spectrum, of  $D_q$  against  $q$ , for a set of  $q$  values (e.g., the integer numbers -8, ..., -1, 0, +1, ..., +8).

Multifractal analysis (MFA) can be applied in the temporal domain, which is 1D and ordered, as well as in the 1D, 2D and 3D spatial domains, which are not ordered. Modern technologies, including but not restricted to computed tomography (CT) scanning and magnetic resonance imaging (MRI), give researchers access to 3D data acquisition in studies in soil and plant sciences and forestry (Ketcham and Carlson, 2001; Dutilleul and Lafond, 2016; Beaulieu and Dutilleul, 2019). The increased availability of such technologies is accompanied by a greater diversity in the format of datasets that needs to be taken into account in the applications of the MFA. Whether the framework is temporal or spatial, uni- or multi-dimensional, and the data are graphical or numerical in nature, it is important that an MFA program be general enough while implementing complicated equations without effort for the user. This is what we have to offer, for the analysis of multi-scale structural complexity along a 1D axis while the whole domain of study is 1D, 2D or 3D. In the rest of the paper, we present the MFA application that we have written in MATLAB programming language (The MathWorks, Inc., Natick, MA, USA), with its possible inputs, mode of execution, and possible outputs; three examples with specific objectives in different areas are presented in the next section (Results and Discussion), followed by a brief Conclusion.

## 2. The MFA program

## 2.1. Program inputs

The MFA program is GUI-based (GUI: Graphical User Interface), and was originally written in MATLAB Version 8.5 (R2015a). It reads input files in a variety of formats, detailed in the User's Guide (see Supplementary Material). Three sets of volumetric (3D) data collected in studies from different sectors of Agriculture (Figure 1) are presented to allow a comprehensive discussion of the execution of the program and the interpretation of its outputs. From Lafond et al. (2012), CT scanning data for a soil column taken from an agricultural field provide the first example, in which porosity is analyzed by MFA from top to bottom of the soil column; one of 500 CT images is shown in Figure 1(a). Duly processed CT scanning data from Dutilleul et al. (2015), on the distribution of branches in the crown of a miniature conifer from bottom to top, provide the second example; see Figure 1(b) for the 3D image of the skeletal branching pattern. Micro-CT scanning data collected in a chapter of the Ph.D. thesis project of Franziska Srocke (McGill-U. of Edinburgh), where pores in softwood pellet biochar are of interest (along one of the three axes of micro-CT scanning chosen as investigation axis; see 2D image in Figure 1c), illustrate a different situation regarding the fractality of the underlying structure. In these three examples, the number of soil pore voxels, the number of branch voxels (with the limit of one pixel for the representation of a branch in a 2D CT image), and the number of biochar pore voxels provide the basis to quantify mass concentration in multifractal terminology, from beginning to end of some range along a preferential axis.

(insert Figure 1 here)

The pseudo-macropore<sub>gas</sub> voxels counted for a given threshold in each cross-sectional CT image (Lafond et al., 2012) were stored in a text (.txt) file for use as input of the MFA program in the soil column example. In the miniature conifer example, the skeletal branching pattern derived from the crown that had been CT scanned (Dutilleul et al., 2015) was reduced to a point pattern (1 point = 1 branch) in each cross-sectional CT image, to avoid any over-representation of a tree branch skeleton in an image that would otherwise lead to an over-estimation of mass concentration in the MFA. The input data are numbers of branch pixels per image, stored as a single column or a single row in a Microsoft Excel (.xls or .xlsx) file. In both these examples, the data can be plotted easily as a curve and the choice for the direction (from top to bottom or vice versa) is natural. The MFA input for the biochar sample example is of graphical instead of numerical nature, as it is a stack of binary images processed from micro-CT images. Figure 1(c) shows one such binary image, where the black area is composed of the biochar pore pixels as pixels of interest. A conversion from image to count is done automatically after a preliminary check of the input data type is made by the program.

## 2.2. Program execution

The MFA program was written and tested on a Dell XPS (CPU: Intel Core i7 3.60 GHz, RAM: 16 GB), with Windows 7 Enterprise as the operating system. After launching it successfully, the user can browse the file system to locate the input data file (Figure 2, INPUT section).

(insert Figure 2 here)

As it is common practice with GUI-based applications, the MFA program produces figures to help grasp the input data characteristics and visualize the results, and the graphical interface has three sections. Following San José Martínez et al. (2010) and Lafond et al. (2012) for the MFA method that is applied, Figure 2 (DISPLAY section) shows the original 1D curve of one input dataset with the basic information about it. After the data range (over which the MFA will actually be performed) is reset by the user, an interpolated curve, with a length equal to the power of 2 the closest to the data range, is displayed. This is to meet a fundamental requirement of fractal analysis (i.e., multiple dyadic divisions made in log-log plots for the estimation of parameters), and cubic spline data interpolation is done automatically by the program, with an accuracy of 0.01 in curve length units; see the User's Guide. Each of the two multifractal spectra can be displayed with the corresponding button click. The MFA program uses default criteria to display points in spectrum plots; some, related to estimation precision, are illustrated with the miniature conifer example (Results and Discussion).

### *2.3. Program outputs*

Users may choose to save one or several output files for further analysis, from a list of graphical or numerical format options in the OUTPUT section (Figure 2). The numerical values saved as output are not submitted to the default criterion of minimum estimation precision  $R^2 > 0.81 = (0.9)^2$  ( $R^2$ : coefficient of determination) used for spectrum plots in the MFA program, which gives more flexibility to users for their own subsequent data analysis or presentation of MFA results. The User's Guide gives details about the structure of the three output Data Tables (Excel files).



### 3. Results and discussion

The datasets used in the three examples presented below come from different agricultural research areas, so no attempt will be made to compare the MFA results between examples. Instead, in each example, the multifractal hypothesis is tested against the monofractal hypothesis for the underlying structure (i.e., soil porosity, tree branching, biochar porosity). In this hypothesis testing, it must be noted that the Rényi dimensions are stationarized by dividing each of them by the monofractal dimension estimated by box counting, so the Rényi dimension for  $q = 0$  is equal to 1.0; a similar standardization is applied to the  $\alpha_q$ 's and  $f(\alpha_q)$ 's, so  $\alpha_0 = 1.0$  and  $f(\alpha_0) = 1.0$ . Besides testing aspects, a main objective is to learn how to interpret the results for the singularity and Rényi spectra because these have specific interpretation rules regarding patterns to be seen in the plots.

#### 3.1. Soil column example

The number of CT images being 500, the number of counts of pseudo-macropore<sub>gas</sub> voxels in the input text file prepared for an MFA is also 500; each count is an estimate of soil porosity in a 0.3-mm cross-section at a given depth inside the soil column, for a certain threshold applied to all the gray-tone CT images (Figure 1a here; see also Lafond et al., 2012). After reading of the file into the MFA program, the original curve is displayed in its entirety (Figure 3, top left). Due to strong surface effects (in the first Input Data) and strong bottom effects (in the last Input Data), where air is over-represented, it is necessary to reset the range (e.g., from 51 to 420 in this case) to avoid these artefacts. The new number of counts being 370, which is greater than the geometric mean (362) of  $256 = 2^8$  and  $512 = 2^9$ , an interpolated curve with same beginning (51) and end (420), but

with 512 data points in total, is computed and plotted (Figure 3, top right). Finally, the singularity and Rényi multifractal spectra are computed on the interpolated data, and plotted as requested (Figure 3, bottom).

(insert Figure 3 here)

The singularity spectrum (Figure 3, bottom left) is asymmetrical, both left-right and top-bottom, and widely dispersed ( $\Delta\alpha > 0.25$ ,  $\Delta f(\alpha) > 0.45$ ), indicating that the soil pore distribution is multifractal rather than monofractal. Specifically, (1) the width  $\Delta\alpha$  of the singularity spectrum is related to the heterogeneity of the curve, that is, the wider the spectrum, the greater the variety of scales of the studied curve, and vice versa; (2) larger concentrations (smaller  $\alpha$ -estimates) are less diverse and more common than smaller concentrations (larger  $\alpha$ -estimates). In the Rényi spectrum (Figure 3, bottom right), the noticeable departure from 1.0 (i.e., the standardized value of  $D_0$ ) indicates heterogeneity in the estimated generalized dimensions, thus supporting multifractality; the discrepancy is greater on the left-hand side ( $q < 0$ ) than on the right-hand side ( $q > 0$ ). In both spectra, the standard errors associated with the multifractal parameter estimates allow the user to assess whether a difference between two values is significant relative to the dispersion.

### 3.2. Miniature conifer example

The 3D skeletal branching pattern of a miniature conifer (Figure 1b) is that of the *Cryptomeria japonica* (Monstrosa Nana) specimen, after its CT scanning and the appropriate processing of the CT images (Dutilleul et al., 2015). Prior to performing the MFA, the original number of 448 cross-

sections is increased to 512 within the selected range for the construction of the interpolated curve from the original curve (Figure 4, top), with the same explanation as for the soil column example. This time, the two curves represent, with 448 and 512 data points, respectively, the density of branches in the crown at successive heights.

(insert Figure 4 here)

The missing points in the multifractal spectra mean that the condition  $R^2 > 0.81$  was not met for the estimation of the abscissa or ordinates, or both, for four positive values of  $q$  in the singularity spectrum (Figure 4, bottom left) and of the generalized dimensions  $D_q$ ,  $q = 1, 2$  (Figure 4, bottom right). For  $D_2$ , for instance, there was a lack of fit in the middle (for intermediate values of the scaling factor) of the log-log plot to be used for its estimation. When encountering such a situation, users may refer to the numerical outputs because these will contain all the estimates, with the corresponding  $R^2$  whether greater than 0.81 or not. Nevertheless, the discrepancies ( $\Delta\alpha > 0.6$ ,  $\Delta f(\alpha) > 0.5$ ,  $|D_q - 1.0|$  as large as 0.3) leads to a conclusion similar to that in the soil column example, i.e., multifractality of the structure and heterogeneity of the mass concentration for tree branching.

### 3.3. Biochar sample example

The MFA program can also read a stack of binary images as input. The volumetric (3D) micro-structure of biochar was stored in the form of 1024 micro-CT images for a sample of a few mm<sup>3</sup>; since  $1024 = 2^{10}$ , no interpolation is required, or original data and interpolated data are the same. Before loading, the 2D micro-CT images are binarized in sequence in accordance with the interest

of the study (i.e., the color black is used to represent the pixels of interest). Then, the 1D curve is computed and displayed by the program. No missing image is allowed in the sequence. Although this type of input may be convenient to users in some cases, it is more time-consuming because of the loading and processing of images.

(insert Figure 5 here)

The singularity and Rényi spectra are very different in this example, compared to the previous examples. For the biochar micro-structure studied along the direction that was chosen, (1) there is almost perfect left-right symmetry around  $\alpha = 1.0$  and a very narrow dispersion ( $\Delta\alpha < 0.0005$ ,  $\Delta f(\alpha) < 0.003$ ) in the singularity spectrum, and (2) the  $D_q$  estimates,  $q = -8, \dots, -1, 0, +1, \dots, +8$ , are almost perfectly aligned on a horizontal straight line passing by (0, 1.0) with  $|D_q - 1.0| < 0.0005$  in the Rényi spectrum, clearly showing homogeneity. In other words, this is an exemplary set of MFA results that support monofractality.

#### **4. Conclusion**

As interest in the MFA method increases over the next few years in soil and plant sciences, as well as other areas of agricultural research and beyond (e.g., the environmental sciences), researchers can rely on the GUI-based application for Windows platforms that we have developed, and present here. It is general and flexible with regards to input and output formats, provides quantitative details and produces graphs for multifractal spectra, and should prove very helpful to many researchers. (A copy of the compiled MFA program, similar to the one provided as Supplementary

Material with the submitted Manuscript, is expected to be posted later at <https://environmetricslab.mcgill.ca>, Computer Programs section, and downloadable free of charge.) The methodology allows a 1D axis of investigation for multi-scale structural complexity.

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## Appendix

In a given (mono- or multi-) fractal system, for a scaling factor  $\varepsilon$  (given by  $2^{-k}L$ , with  $k = 0, 1, 2, \dots$  and  $L$ , the length of the interval over which the analysis is to be performed) and the probability measure of interest  $\mu$ , the singularity strength  $\alpha$  for subinterval  $I_i(\varepsilon)$  is provided by

$$\alpha_i(\varepsilon) = \frac{\log \mu_i(\varepsilon)}{\log \varepsilon} .$$

Larger values of  $\alpha$  mean less concentrated measures, and vice versa. Then, the number of subintervals  $N(\alpha)$  with singularity strength between  $\alpha$  and  $\alpha+d\alpha$  can be approximated by

$$N_\varepsilon(\alpha) \approx \varepsilon^{-f(\alpha)} ,$$

where  $f(\alpha)$  is called “singularity spectrum” (Chhabra and Jensen, 1989; Evertsz and Mandelbrot, 1992).

The three equations below are key for the estimation of singularity spectra:

$$f(\alpha_q) = \lim_{\varepsilon \rightarrow 0} \frac{\sum_{i=1}^{n(\varepsilon)} \mu_i(q, \varepsilon) \log \mu_i(q, \varepsilon)}{\log \varepsilon} ,$$

$$\alpha(q) = \lim_{\varepsilon \rightarrow 0} \frac{\sum_{i=1}^{n(\varepsilon)} \mu_i(q, \varepsilon) \log \mu_i(\varepsilon)}{\log \varepsilon} \quad \text{and}$$

$$\mu_i(q, \varepsilon) = \frac{\mu_i(\varepsilon)^q}{\sum_{i=1}^{n(\varepsilon)} \mu_i(\varepsilon)^q},$$

where  $n(\varepsilon)$  denotes the number of subintervals at scale  $\varepsilon$  obtained by dyadic downscaling of the original interval, and  $q$  is a predefined set of real numbers in theory and a predefined subset of negative and positive integer numbers symmetric with respect to 0 in practice. The Hölder exponent  $\alpha$  is therefore a decreasing function of  $q$ . For  $q > 1$ , smaller values of  $\alpha$  mean greater concentrations of the probability measure, and vice versa.

Generalized dimensions, called “Rényi dimensions” (Grassberger, 1983), provide an alternative multifractal spectrum, and are defined by:

$$D_q = \frac{1}{q-1} \lim_{\varepsilon \rightarrow 0} \frac{\log \sum_{i=1}^{n(\varepsilon)} \mu_i(\varepsilon)^q}{\log \varepsilon} \quad \text{for } q \neq 1 \quad \text{and}$$

$$D_1 = \lim_{\varepsilon \rightarrow 0} \frac{\sum_{i=1}^{n(\varepsilon)} \mu_i(\varepsilon) \log \mu_i(\varepsilon)}{\log \varepsilon} \quad \text{when } q = 1.$$

In general, Rényi spectra are monotonic-decreasing and sigmoid-shaped. The more horizontal a Rényi spectrum is, the less there is evidence favoring multifractality over monofractality. By comparison, singularity spectra have a convex shape and the span and symmetry of the points  $(\alpha(q), f(\alpha_q))$  reveal the characteristics of the fractal system; a very clustered display is expected for a homogenous monofractal system. See San José Martínez et al. (2010) and Lafond et al. (2012) for more details.



## Figure captions

Figure 1. Left panel, Example of 2D CT image for a soil column taken from an agricultural field. Middle panel, 3D image of the skeletal branching pattern of a miniature conifer, constructed from CT scanning data. Right panel, Example of binary 2D micro-CT image showing the interior part of a softwood pellet biochar sample.

Figure 2. Interface of the MFA program, with three sections: INPUT, to Load data from an input file; OUTPUT, with seven possible choices of output file format after a string is entered as prefix for the output file name(s); and DISPLAY, for a plot of the data, original or interpolated, or the multifractal spectrum of singularity or Rényi, with the coordinates of the two co-developers.

Figure 3. The four possible figure outputs (original data, interpolated, singularity spectrum, Rényi spectrum, from left to right and top to bottom) for the soil column example.

Figure 4. The four figure outputs for the miniature conifer example.

Figure 5. The four figure outputs for the biochar sample example.